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A RAPID CALCULATIONAL METHOD FOR MULTIGROUP ELASTIC TRANSFER*

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ABSTRACT

Continuous slowing down theory is applied to the generation of elastic transfer matrices at the broad group level. When incorporated into a standard processing code, substantial savings in time were achieved while retaining acceptable accuracy.

Calculation of elastic transfer matrices can be a time-consuming component of processing nuclear data to obtain multigroup constants. In an attempt to reduce computing costs, we attempted to find an alternate calculational procedure which is inexpensive, reasonably accurate, and easily implemented. The three objectives were realized through use of continuous slowing down theory. Other approaches to this problem also have been suggested (1).

Let us consider first why the problem of time-consumption arises. Elastic transfer cross-sections involve integrals of the general form (2)

$$I_k = \int du' \int du'' \, \phi_k(u') P_k[\mu_o(U)] \left(-\frac{d\mu_c}{dU}\right) \sum_{k'=0}^{K} \frac{2k'+1}{2} \sigma^c_{gk'}(u') P_{k'}[\mu_c(U)] \qquad (1)$$

In Equation 1, the k-index denotes the Legendre moment in the laboratory system, and the k' index is used for the summation of center-of-mass system components of the cross-section. Evaluation of Equation 1 can be time-consuming because the Legendre moments Pk(μ) are rapidly fluctuating functions. The scattering angle cosines in laboratory and center of mass μ_o and μ_c both are functions of the lethargy change U.

The expense associated with Equation 1 is compounded by the number of integrals to be evaluated. Suppose, for example, that one is dealing with about [illegible] groups and P8 scattering, and that scattering to only one lower group is possible. We thus have to perform about four hundred fifty double integrals. Each integral would involve a considerable number of operations because of the large number of integration points and the summation within the integral.

To see how continuous slowing down theory can help the situation, let us first consider the case in which downscatter to only one group is permitted. If one takes Taylor expansions for collision density terms within integrands,

and retains only the leading terms, the slowing down density for the kth Legendre moment is (2)

$$\rho_k(u_g) = \sum_{k'=0}^{K} \xi_{kk'} \sigma^c_{sk'}(u_g)\, \phi_k(u_g) \tag{2}$$

where slowing down parameters are defined for the various Legendre moments

$$\xi_{kk'} = \frac{2k'+1}{2} \int_{-1}^{1} P_k[\mu_0(\mu_c)]\, U(\mu_c) P_{k'}(\mu_c)\, d\mu_c \tag{3}$$

Since all neutrons slowing down past a group boundary enter the next group, the removal cross-section can be related to the slowing down density by

$$\rho_k(u_g) = \sigma_k^{g\to g+1}\, \phi_k^g \tag{4}$$

From the above, the removal cross-section is given by

$$\sigma_k^{g\to g+1} = \frac{\phi_k(u_g)}{\phi_k^g} \sum_{k'=0}^{K} \xi_{kk'} \sigma^c_{sk'}(u_g) \tag{5}$$

The numerical gain in using Equation 5 is clear. First, the only single integral involved is $\xi_{kk'}$ which is independent of group, and the integration work is insensitive to the number of groups. This is in contrast to the large number of double integrals normally required. The ratio of the flux at the bottom of the group to the total group flux would be obtained easily from the weighting spectrum used.

The in-group scattering cross-section can be obtained in terms of Equation 5 and the total scattering cross-section, which is given by

$$\sigma^g_{sk} = \frac{1}{\phi_k^g} \int_{u_{g-1}}^{u_g} du\, \phi_k(u) \sum_{k'} T_{kk'} \sigma^c_{sk'}(u) \tag{6}$$

$$T_{kk'} = \frac{2k'+1}{2} \int_{-1}^{1} d\mu_0 \, P_k [\mu_0(\mu_c)] \, P_{k'}(\mu_c) \tag{7}$$

The in-group scattering is given by

$$\sigma_k^{g \to g} = \sigma_{sk}^{g} - \sigma_k^{g \to g+1} \tag{8}$$

The above procedure was incorporated into the SUPERTOG code (3) to replace the existing elastic transfer calculation. Overall code running time was reduced by about a factor of eight for the problems considered. In essence, a transition was achieved from a situation where running time was determined by elastic matrices to a situation where running time was determined by other aspects of cross-section processing. Some results are shown in Table I at high energy where several orders of anisotropy are substantial. Results here and in the other applications we have considered are acceptable in accuracy, while being achieved at a substantial saving in computer time.

The limitation to single group downscatter is applicable to many realistic situations and is present in commonly used calculations (4). However, it would be desirable to remove this limitation if possible. The difficulty with applying continuous slowing down theory to multigroup transfer is that continuous slowing down concepts generally are associated with a single lethargy or energy. Thus, the slowing down density past a given lethargy could be translated into a removal cross-section as long as it is known that downscatter to only one group is possible.

To circumvent this difficulty, we shall make use of the techniques utilized in deriving continuous slowing down theory, rather than the currently used concepts. In particular, we shall make use of Taylor series expansions of collision

densities in the integrals for the group constants.

Let us consider a situation where scattering down to two groups is possible. The two-group transfer cross-section is

$$\sigma_k^{g\to g+2} = \frac{1}{\phi_k^g}\int_{u_{g+1}-\epsilon}^{u_g} du' \int_{u_{g+1}}^{u'+\epsilon} du'' \left(-\frac{d\mu_c}{dU}\right) \phi_k(u') P_k\left[\mu_0(U)\right] \sum_{k'=0}^{K} \frac{2k'+1}{2} \sigma_{sk'}^{c}(u') P_{k'}\left[\mu_c(U)\right] \quad (9)$$

$$\epsilon = \ln\frac{1}{\alpha} \quad (10)$$

Now consider Taylor expansions of the form

$$\sigma_{sk'}^{c}(u')\,\phi_k(u') = \sigma_{sk'}^{c}(u_g)\,\phi_k(u_g) + (u'-u)\frac{d}{du_g}\left[\sigma_{sk'}(u_g)\,\phi_k(u_g)\right] + \cdots \quad (11)$$

To date, only the first term in the expansion, analogous to the Fermi age approximation, has been considered. Equation 9 then becomes

$$\sigma_k^{g\to g+2} = \frac{\phi_k(u_g)}{\phi_k^g} \sum_{k'=0}^{K} \frac{2k'+1}{2} \sigma_{sk'}^{c}(u_g) \int_{u_{g+1}-\epsilon}^{u_g} du' \int_{u_{g+1}}^{u'+\epsilon} du'' P_k\left[\mu_0(U)\right] P_{k'}\left[\mu_c(U)\right] \left(-\frac{d\mu_c}{dU}\right) \quad (12)$$

Equation 12 can be expressed in a manner analogous to that of Equation 5

$$\sigma_k^{g\to g+2} = \frac{\phi_k(u_g)}{\phi_k^g} \sum_{k'=0}^{K} \zeta_{kk'}^{g\to g+2}\, \sigma_{sk'}^{c}(u_g) \quad (13)$$

$$\zeta_{kk'}^{g\to g+2} = \frac{2k'+1}{2} \int_{u_{g+1}-\epsilon}^{u_g} du' \int_{u_{g+1}}^{u'+\epsilon} du'' P_k\left[\mu_0(U)\right] P_{k'}\left[\mu_c(U)\right] \left[-\frac{d\mu_c}{dU}\right] \quad (14)$$

If the group widths are uniform, we again have a situation where the integrations are performed once and then used for all groups. Note that the approach yields slowing down parameters $\zeta_{kk'}^{g\to g+2}$ associated with transfer to particular lethargy

ranges rather than total slowing down parameters as usually encountered in continuous slowing down theory.

Equation 14 as written is a double integral, which makes it less convenient to evaluate than Equation 3, a single integral. However, Equation 14 can be converted to a single integral by a simple procedure (5). Note that all terms in the integrand are functions of the lethargy change U. Denoting the integrand by $f(U)$ for simplicity, it is logical to change variables to obtain

$$\xi_{kk'}^{g\to g+2} = \int_{u_{g+1}-\epsilon}^{u_g} du' \int_{u_{g+1}}^{u'+\epsilon} du'' f(U) = \int_{u_{g+1}-\epsilon}^{u_g} du' \int_{u_{g+1}-u'}^{\epsilon} dU\, f(U) \tag{15}$$

Reversing the order of integration leads to

$$\xi_{kk'}^{g\to g+2} = \int_{\Delta_g}^{\epsilon} dU\, f(U) \int_{u_{g+1}-U}^{u_g} du' \tag{16}$$

$$\Delta_g = u_{g+1} - u_g \tag{17}$$

The integral over u' can be performed analytically, yielding

$$\xi_{kk'}^{g\to g+2} = \frac{2k'+1}{2} \int_{\Delta_g}^{\epsilon} dU\, (U-\Delta_g) P_k[\mu_0(U)] P_{k'}[\mu_c(U)] \left(-\frac{d\mu_c}{dU}\right) \tag{18}$$

Equation 18 can be converted to an integral over center of mass angle, analogous to Equation 3,

$$\xi_{kk'}^{g\to g+2} = \frac{2k'+1}{2} \int_{-1}^{\mu_c(\Delta_g)} d\mu_c\, [U(\mu_c)-\Delta_g] P_k[\mu_0(\mu_c)] P_{k'}(\mu_c) \tag{19}$$

$$\mu_c(\Delta_g) = 1 - \frac{(A+1)^2}{2A}\left(1 - e^{-\Delta_g}\right) \tag{20}$$

Analogous expressions can be derived directly for downscattering one group. On the other hand, one can infer the one-group downscatter from the total slowing down density and the two group downscatter.

$$\sigma_k^{g\to g+1} = \frac{\phi_k(u_g)}{\phi_k^g} \sum_{k'=0}^{K} \left(\xi_{kk'} - \xi_{kk'}^{g\to g+2} \right) \sigma_{sk'}^{c}(u_g) - \frac{\phi_k(u_{g-1})}{\phi_k^g} \sum_{k'=0}^{K} \xi_{kk'}^{g-1\to g+1} \sigma_{sk'}^{c}(u_{g-1}) \quad (21)$$

Two terms have to be subtracted. One is due to the fact that two group scattering from group "g" is possible. The second is due to the fact the slowing down density at lethargy u_g has a contribution from group "g-1."

In single group transfer, only one set of integrals independent of group had to be evaluated. Equation 19 for two-group transfer obviously has to depend on the width of the intervening group. However, it should not be necessary to increase significantly the integration effort. Equation 19 may be written as

$$\xi_{kk'}^{g\to g+2} = \int_{-1}^{\mu_c(\Delta_g)} d\mu_c\, f_1(\mu_c) - \Delta_g \int_{-1}^{\mu_c(\Delta_g)} d\mu_c\, f_2(\mu_c) = I_1 - \Delta_g I_2 \quad (22)$$

Suppose there are N group widths of interest. One then can write, for example,

$$I_1 = \int_{-1}^{\mu_c(\Delta_{g,1})} d\mu_c\, f_1(\mu_c) + \int_{\mu_c(\Delta_{g,1})}^{\mu_c(\Delta_{g,2})} d\mu_c\, f_1(\mu_c) + \cdots + \int_{\mu_c(\Delta_{g,N-1})}^{\mu_c(\Delta_{g,N})} d\mu_c\, f_1(\mu_c) \quad (23)$$

or, symbollically

$$I_1 = I_1^1 + I_1^2 + \cdots + I_1^N \quad (24)$$

Thus, substantial duplication of calculational effort is not necessary to deal with non-uniform group structure. Extension to three or more group transfer is straightforward.

In our own application of this procedure we permit two group sizes, one for which two-group downscatter is possible, and one for which one-group downscatter only is possible. This is in keeping with analysis of fast spectrum measurements at RPI. Incorporation of the technique into SUPERTOG again led to a gain of a factor of about eight in overall running time of the code. Some sample results are given in Table 2. Again, reasonable accuracy has been obtained.

It should be noted that this approach is particularly attractive in connection with parametric generation of elastic matrices in terms of background cross-sections (4). In such parametric generation, one is interested in scalar weighting spectra of the form

$$\phi_0(u) = \frac{1}{\sigma_{tr}(u) + \sigma_0} \tag{25}$$

Equation 5 would become, for example,

$$\sigma_0^{g \to g+1}(\sigma_0) = \frac{\frac{1}{\sigma_{tr}(u_g) + \sigma_0}}{\int_{u_{g-1}}^{u_g} \frac{du}{\sigma_{tr}(u) + \sigma_0}} \sum_{k'=0}^{K} \xi_{0k'} \sigma_{Sk'}^{c}(u_g) \tag{26}$$

Note that the summation over the k' index does not involve the background cross-section. The only integral to be evaluated for each case is the group flux

$$\phi_0^g = \int_{u_{g-1}}^{u_g} \frac{du}{\sigma_{tr}(u) + \sigma_0} \tag{27}$$

Henryson (5) has obtained similar expressions to ours for downscatter cross-sections, though his motivation, assumptions, and application differ from ours. He was concerned with reliably obtaining elastic transfer cross sections on an ultra-fine level (group lethargy width of 1/120) for heavy elements, such as uranium. He assumed that for groups so narrow, the cross-sections and flux in

(for example) Equation 9 could be replaced by the average values of these quantities for the group. He thus obtains the same integrals to evaluate as obtained above, but his coefficients will differ if the average values of cross-sections and weighting spectra differ from values at the bottoms of groups. Our concern has been with fairly broad groups (group lethargy widths of 1/8 and 1/4) for direct input into transport or diffusion calculation, and with light and intermediate mass materials in addition to heavy materials.

In summary, a rapid and easily implemented procedure has been formulated for generating elastic matrices. The procedure has been incorporated into a standard cross-section processing code, leading to a substantial saving of running time with retention of acceptable accuracy.

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TABLE 1

Comparison of New and Standard Group Constants from SUPERTOG for Elastic Scattering from Group 4 (5.35-6.87 MeV, $\Delta u = .125$) using ENDF/B-I Iron Data

	$\sigma_{4\to4}$			$\sigma_{4\to5}$	
Legendre Moment	New	Standard	Legendre Moment	New	Standard
0	2.37	2.37	0	.133	.132
1	1.81	1.81	1	.0253	.0248
2	1.34	1.34	2	.0131	.0133
3	.934	.938	3	.00901	.00856
4	.556	.557	4	-.00729	-.00684
5	.287	.288	5	-.00118	-.00110
6	.141	.141	6	-.00438	-.00468
7	.0673	.0692	7	-.000962	-.00115
8	.0275	.0296	8	-.00177	-.00159

TABLE 2

Selected Isotropic Elastic Group Constants for Sodium ($\Delta u = .125$)

	Fast CSD Method	Standard SUPERTOG
$\sigma^{47\to47}$	1.89	1.88
$\sigma^{47\to48}$	2.89	2.90
$\sigma^{47\to49}$	.28	.28
$\sigma^{46\to46}$	1.82	1.81
$\sigma^{46\to47}$	2.78	2.80
$\sigma^{46\to48}$	.27	.26
$\sigma^{45\to45}$	1.75	1.75
$\sigma^{45\to46}$	2.71	2.72
$\sigma^{45\to47}$	.26	.26
$\sigma^{44\to44}$	1.71	1.70
$\sigma^{44\to45}$	2.64	2.65
$\sigma^{44\to46}$	.26	.25